SYNTHESIS AND STRUCTURE OF BIS(PHENYLTETRAMETHYLCYCLOPENTADIENYL)TITANIUM(III) HYDRIDE - THE FIRST MONOMERIC BIS(CYCLOPENTADIENYL)TITANIUM(III) HYDRIDE

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Abstract. "IUPAC-name", $C_{30}H_{35}Ti$, M_r = 443.49, triclinic, $P\bar{1}$, a = 9.097(1), b = 12.102(1), c = 12.317(1) Å, α = 76.646(4)°, β = 72.618(4)°, γ = 69.643(4)°, V = 1201.0(2) Å^3, Z = 2, D_X = 1.226 g cm^{-3}, λ(Mo $K\bar{\alpha}$) = 0.71073 Å, μ = 3.65 cm^{-1}, $F(000)$ = 474, T = 130 K, R_F = 0.033 for 4633 unique observed reflections with $I \geq 2.5\ \sigma(I)$ and 422 parameters.
The interatomic Ti-H(1) distance is 1.768(15) Å.

Experimental.

X-ray diffraction: Crystal and Molecular Structure.

X-ray quality crystals of the title compound were obtained directly from the preparations as described above. The red colored crystal, a parallelepiped of approximate size 0.22 x 0.34 x 0.42 mm., used for characterization and data collection, was glued on a glass fiber and transferred to the goniostat by using inert-atmosphere handling techniques and cooled to 130 K by using an on-line liquid nitrogen cooling system[1] mounted on an Enraf-Nonius CAD-4F diffractometer interfaced to a MicroVAX-2000 computer. Unit cell parameters were determined from a least-squares treatment of the SET4[2] setting angles of 22 reflections from various parts of reciprocal space, with 17.83° < θ < 20.69°. The unit cell was identified as triclinic, space group $P\bar{1}$. This assignment was confirmed by the solution and the successful refinement. Reduced cell calculations did not indicate any higher metric lattice symmetry[3] and examination of the final atomic coordinates of the structure did not yield extra metric symmetry elements.[4,5] The intensities of the three standards reflections, measured every three hours of X-ray exposure time, showed no greater fluctuations during data collection than those expected from Poisson statistics. Intensity data were corrected for Lorentz and polarization effects, scale variation and reduced to F_O.[6] Absorption correction was judged not to be necessary in view of the small observed variation in intensity (5% about the mean value) of a 360° ψ-scan of a close-to-axial reflection ($\bar{2}\bar{2}2$). Variance was calculated based on counting statistics and the term (P^2I^2) where P (= 0.0176) is the instability constant[7] as derived from the excess variance in the reference reflections. Equivalent reflections were averaged and stated observed if satisfying the $I \geq 2.5\ \sigma(I)$ criterion of observability.

The structure was solved by Patterson methods and extension of the model was accomplished by direct methods applied to difference structure factors using the program *DIRDIF*.[8] The positional and anisotropic thermal displacement parameters for the non-hydrogen atoms were refined with block-diagonal least-squares procedures (*CRYLSQ*)[9] minimizing the function $Q = \Sigma_h\ [w(|F_O| - k|F_C|)^2]$, where the weight w is defined as $1/\sigma^2(F)$ and F_O and F_C are the observed and calculated structure factor amplitudes, respectively. Subsequent difference Fourier synthesis resulted in the location of all the hydrogen atoms, which positions were included in the refinement. Weights were introduced in the final refinement cycles. The crystal exhibited some secondary extinction for which the F_C values were corrected by refinement of an empirical isotropic extinction parameter.[10] Refinement on F_O by full-

matrix least-squares techniques with anisotropic thermal displacement parameters for the non-hydrogen atoms and isotropic thermal displacement parameters for the hydrogen atoms converged at $R_F = 0.033$ ($wR = 0.041$). A final difference Fourier map did not show residual peaks outside the range ±0.30 e/Å^3.

Crystal data and experimental details of the structure determination are compiled in Table 1. Final fractional atomic coordinates and equivalent isotropic thermal displacement parameters for the non-hydrogen atoms are given in Table 2. Molecular geometry data are collected in Table 3. Tables of hydrogen atom positions, thermal displacement parameters, comprehensive lists of bond distances and angles and tables of (F_O), (F_C) and σ(F) are given as supplementary material* for this paper. Neutral atom scattering factors[11] were used and anomalous dispersion factors[12] were included in F_C. All calculations performed (were carried out) on the HP9000/735 computer at the University of Groningen with the program packages *Xtal*,[13] *PLATON*[14] (calculation of geometric data) and a locally modified version of the program *PLUTO*[15] (preparation of illustrations).

Results and discussion.

The identification of the atoms and the configuration are shown in the *PLUTO* drawing of Fig. 1.; the packing of the molecules is shown in the unit cell in Fig. 2. The triclinic unit cell contains two discrete molecules (Fig. 2) of the title compound separated by normal van der Waals distances.[17]

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* **Supplementary Material:** Tables of crystal data, anisotropic thermal displacement parameters, atomic coordinates, bond lengths, bond angles, and torsion angles (.. pages) and an *ORTEP*[16] plot; a listing of observed and calculated structure factors (.. pages). Ordering information is given on any current masthead page.

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Table 1.

a. Crystal data and details of the structure determination.

Chemical formula	$C_{30}H_{35}Ti$
Formula weight, g.mol^{-1}	443.49
Crystal system	triclinic
Space group, no.[18]	$P\bar{1}$, 2
a, Å	9.097(1)
b, Å	12.102(1)
c, Å	12.317(1)
α, deg	76.646(4)
β, deg	72.618(4)
γ, deg	69.643(4)
V, Å^3	1201.0(2)
Z	2
D_{calc}, g.cm^{-3}	1.226
F(000), electrons	474
μ(Mo $K\bar{\alpha}$), cm^{-1}	3.65
Approx. crystal dimension, mm	0.22 x 0.34 x 0.42

b. Data collection.

Radiation	Mo $K\bar{\alpha}$
Wavelength, Å	0.71073
Monochromator	Graphite
Temperature, K	130
θ range; min. max., deg	1.75, 27.0
ω/2θ scan, deg	$\Delta\omega = 0.75 + 0.34$ tg θ
Data set	h: -11→11; k: -15→15; l: 0→15
Crystal-to-receiving-aperture distance, mm	173
Horizontal, vertical aperture, mm	3.2 + tg θ; 4.0
Reference reflections, r.m.s. dev. in %	$0\bar{3}1$, 1.0 $\bar{2}10$, 1.0 $\bar{1}\bar{2}3$, 0.7
Instability constant, P	0.0176
Drift correction	0.993 - 1.000
X-ray exposure time, h	64.3
Total data	5483
Unique data	5324
Observed data ($I \geq 2.5\ \sigma(I)$)	4633
$R1$ ($= \Sigma(I-\bar{I})/\Sigma I$)	0.009
$R2$ ($= \Sigma\sigma/\Sigma I$)	0.021
Number of equivalent reflections	498

c. Refinement.

Number of reflections	4633
Number of refined parameters	422
Isotropic secondary-extinction coefficient, *g*	$0.27(3)*10^{-4}$
Final agreement factors:	
$R_F = \Sigma(\lvert\lvert F_O\rvert-\lvert F_C\rvert\rvert)/\Sigma\lvert F_O\rvert$	0.033
$wR = [\Sigma(w(\lvert F_O\rvert-\lvert F_C\rvert)^2)/\Sigma w\lvert F_O\rvert^2]^{1/2}$	0.041
Weighting scheme	$1/\sigma^2(F)$
$S = [\Sigma w(\lvert F_O\rvert-\lvert F_C\rvert)^2/(m-n)]^{1/2}$	3.21(3)
m = number of observations	
n = number of variables	
Min. and max. residual densities difference Fourier map, e/Å^3	-0.29, 0.37
Max. (shift/σ) final cycle	$0.3717*10^{-1}$
Average (shift/σ) final cycle	$0.3923*10^{-2}$

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Table S2. Final Fractional Atomic Coordinates and Equivalent Isotropic Thermal Displacement Parameters for non-H Atoms with e.s.d.'s in parentheses.

for: C30H35Ti CP282

Atom	x/a	y/b	z/c	U(eq) [Ang**2]
Ti(1)	0.23717(3)	0.24285(2)	0.21492(2)	0.0171(1)
C(1)	0.36522(17)	0.34010(13)	0.28732(13)	0.0197(4)
C(2)	0.48414(17)	0.23387(13)	0.24926(13)	0.0201(4)
C(3)	0.50755(16)	0.24573(13)	0.12867(13)	0.0195(4)
C(4)	0.40262(17)	0.35651(13)	0.09101(12)	0.0184(4)
C(5)	0.31304(17)	0.41502(12)	0.18928(12)	0.0183(4)
C(6)	0.32304(19)	0.37438(14)	0.40475(14)	0.0262(5)
C(7)	0.57682(19)	0.13231(14)	0.32208(14)	0.0269(5)
C(8)	0.62842(18)	0.15729(14)	0.05285(14)	0.0275(5)
C(9)	0.39707(18)	0.40720(13)	-0.03148(13)	0.0232(4)
C(10)	0.19612(17)	0.53638(12)	0.18678(13)	0.0194(4)
C(11)	0.07264(18)	0.56925(13)	0.12990(14)	0.0235(4)
C(12)	-0.03511(19)	0.68362(14)	0.12582(15)	0.0294(5)
C(13)	-0.0213(2)	0.76697(14)	0.17931(16)	0.0317(5)
C(14)	0.1009(2)	0.73652(14)	0.23543(14)	0.0287(5)
C(15)	0.20888(18)	0.62219(13)	0.23911(13)	0.0230(5)
C(16)	0.05147(17)	0.13979(12)	0.24114(13)	0.0198(4)
C(17)	-0.04057(17)	0.25606(13)	0.26952(13)	0.0219(4)
C(18)	-0.00225(17)	0.27039(13)	0.36730(13)	0.0228(4)
C(19)	0.11238(18)	0.16294(13)	0.40212(13)	0.0218(4)
C(20)	0.14783(17)	0.08289(12)	0.32253(12)	0.0194(4)
C(21)	0.03315(19)	0.08270(14)	0.15208(15)	0.0260(5)
C(22)	-0.16290(19)	0.34555(14)	0.20916(16)	0.0308(5)
C(23)	-0.0785(2)	0.37968(15)	0.42696(15)	0.0327(5)
C(24)	0.1710(2)	0.13237(14)	0.51044(14)	0.0288(5)
C(25)	0.26880(17)	-0.03681(13)	0.32244(13)	0.0206(4)
C(26)	0.39102(19)	-0.06514(14)	0.22341(14)	0.0266(5)
C(27)	0.5093(2)	-0.17515(16)	0.22318(17)	0.0362(6)
C(28)	0.5071(2)	-0.25798(15)	0.32143(19)	0.0409(6)
C(29)	0.3861(2)	-0.23192(14)	0.41899(17)	0.0363(6)
C(30)	0.26691(19)	-0.12238(14)	0.42004(14)	0.0261(5)

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-Hydrogen- parameters:

Atom	x/a	y/b	z/c	U(eq) [Ang**2]
H(1)	0.2593(17)	0.2119(13)	0.0765(13)	0.015(4)
H(6)	0.3924(19)	0.4188(14)	0.4104(15)	0.028(5)
H(6')	0.338(2)	0.3097(16)	0.4625(16)	0.039(5)
H(6")	0.213(2)	0.4271(14)	0.4258(15)	0.029(5)
H(7)	0.525(2)	0.1337(17)	0.4001(17)	0.046(6)
H(7')	0.679(2)	0.1380(18)	0.3175(19)	0.055(6)
H(7")	0.596(2)	0.0564(17)	0.2969(18)	0.055(6)
H(8)	0.661(2)	0.0815(16)	0.0919(17)	0.046(6)
H(8')	0.586(2)	0.1505(18)	-0.0087(18)	0.056(6)
H(8")	0.730(2)	0.1739(17)	0.0209(18)	0.050(6)
H(9)	0.399(2)	0.4849(18)	-0.0472(18)	0.056(6)
H(9')	0.305(2)	0.3992(17)	-0.0537(18)	0.049(6)
H(9")	0.479(2)	0.3715(17)	-0.0820(18)	0.052(6)
H(11)	0.0606(19)	0.5116(15)	0.0932(15)	0.030(5)
H(12)	-0.1192(19)	0.7063(14)	0.0837(14)	0.025(4)
H(13)	-0.099(2)	0.8471(16)	0.1758(16)	0.040(5)
H(14)	0.114(2)	0.7960(16)	0.2717(16)	0.040(5)
H(15)	0.297(2)	0.5997(14)	0.2777(15)	0.029(5)
H(21)	0.131(2)	0.0264(18)	0.1169(18)	0.054(6)
H(21')	-0.050(2)	0.0435(16)	0.1874(17)	0.047(6)
H(21")	0.005(2)	0.1355(17)	0.0899(18)	0.051(6)
H(22)	-0.178(2)	0.4321(17)	0.2150(17)	0.049(6)
H(22')	-0.261(2)	0.3376(18)	0.2423(18)	0.055(6)
H(22")	-0.133(3)	0.3384(18)	0.1267(19)	0.060(7)
H(23)	-0.054(2)	0.4502(16)	0.3785(17)	0.043(6)
H(23')	-0.191(2)	0.3928(17)	0.4553(18)	0.056(6)
H(23")	-0.046(2)	0.3716(19)	0.4955(19)	0.059(7)
H(24)	0.164(2)	0.1960(16)	0.5394(16)	0.041(5)
H(24')	0.1053(19)	0.0859(14)	0.5755(15)	0.027(5)
H(24")	0.281(2)	0.0847(15)	0.5013(15)	0.033(5)
H(26)	0.3960(19)	-0.0049(14)	0.1520(15)	0.028(5)
H(27)	0.589(2)	-0.1897(15)	0.1567(16)	0.040(5)
H(28)	0.593(2)	-0.3327(16)	0.3226(17)	0.047(6)
H(29)	0.380(2)	-0.2885(15)	0.4905(16)	0.037(5)
H(30)	0.1832(19)	-0.1076(14)	0.4869(14)	0.026(4)

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Table S3. Thermal Displacement Parameters with e.s.d.'s in parentheses.
for: C30H35Ti CP282

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Ti(1)	0.0172(1)	0.0187(1)	0.0159(1)	-0.0030(1)	-0.0021(1)	-0.0074(1)
C(1)	0.0201(7)	0.0203(7)	0.0208(7)	-0.0050(6)	-0.0058(6)	-0.0066(6)
C(2)	0.0175(7)	0.0221(7)	0.0224(8)	-0.0053(6)	-0.0059(6)	-0.0058(6)
C(3)	0.0157(7)	0.0220(7)	0.0219(8)	-0.0057(6)	-0.0028(6)	-0.0068(6)
C(4)	0.0178(7)	0.0206(7)	0.0188(7)	-0.0038(6)	-0.0016(6)	-0.0099(6)
C(5)	0.0187(7)	0.0184(7)	0.0195(7)	-0.0039(6)	-0.0030(6)	-0.0082(6)
C(6)	0.0322(8)	0.0266(8)	0.0214(8)	-0.0060(6)	-0.0096(7)	-0.0064(7)
C(7)	0.0240(8)	0.0271(8)	0.0282(9)	-0.0041(7)	-0.0107(7)	-0.0022(6)
C(8)	0.0208(7)	0.0298(8)	0.0279(9)	-0.0105(7)	-0.0021(6)	-0.0018(6)
C(9)	0.0255(8)	0.0249(8)	0.0185(7)	-0.0021(6)	-0.0018(6)	-0.0102(6)
C(10)	0.0206(7)	0.0186(7)	0.0178(7)	-0.0027(5)	0.0003(6)	-0.0084(6)
C(11)	0.0249(8)	0.0219(7)	0.0252(8)	-0.0046(6)	-0.0053(6)	-0.0086(6)
C(12)	0.0247(8)	0.0267(8)	0.0342(9)	-0.0022(7)	-0.0084(7)	-0.0048(7)
C(13)	0.0316(9)	0.0196(8)	0.0362(10)	-0.0053(7)	-0.0023(7)	-0.0023(7)
C(14)	0.0356(9)	0.0212(8)	0.0283(9)	-0.0081(6)	-0.0002(7)	-0.0108(7)
C(15)	0.0259(8)	0.0233(8)	0.0209(8)	-0.0045(6)	-0.0022(6)	-0.0106(6)
C(16)	0.0176(7)	0.0183(7)	0.0227(8)	-0.0005(6)	-0.0030(6)	-0.0074(6)
C(17)	0.0168(7)	0.0190(7)	0.0261(8)	-0.0008(6)	-0.0010(6)	-0.0058(6)
C(18)	0.0199(7)	0.0205(7)	0.0227(8)	-0.0040(6)	0.0036(6)	-0.0062(6)
C(19)	0.0218(7)	0.0225(7)	0.0180(7)	-0.0023(6)	0.0013(6)	-0.0082(6)
C(20)	0.0192(7)	0.0185(7)	0.0186(7)	-0.0005(6)	-0.0014(6)	-0.0073(6)
C(21)	0.0267(8)	0.0242(8)	0.0314(9)	-0.0017(6)	-0.0117(7)	-0.0103(6)
C(22)	0.0202(8)	0.0250(8)	0.0428(10)	0.0020(7)	-0.0091(7)	-0.0046(6)
C(23)	0.0307(9)	0.0260(8)	0.0328(9)	-0.0104(7)	0.0051(7)	-0.0049(7)
C(24)	0.0358(9)	0.0303(8)	0.0181(8)	-0.0047(6)	-0.0024(7)	-0.0100(7)
C(25)	0.0211(7)	0.0180(7)	0.0257(8)	-0.0031(6)	-0.0081(6)	-0.0075(6)
C(26)	0.0260(8)	0.0239(8)	0.0299(9)	-0.0080(7)	-0.0059(7)	-0.0055(6)
C(27)	0.0277(9)	0.0334(9)	0.0478(11)	-0.0200(8)	-0.0110(8)	0.0011(7)
C(28)	0.0384(10)	0.0230(8)	0.0658(14)	-0.0132(9)	-0.0295(10)	0.0042(7)
C(29)	0.0452(10)	0.0220(8)	0.0490(11)	0.0058(8)	-0.0295(9)	-0.0105(7)
C(30)	0.0281(8)	0.0235(8)	0.0305(9)	0.0017(6)	-0.0124(7)	-0.0112(6)

*) The Temperature Factor has the Form of Exp(-T)

Where

T = 8*(Pi**2)*Uiso*(Sin(Theta)/Lambda)**2, for Isotropic Atoms

T = 2*(Pi**2) (Sum(i,j) (h(i)*h(j)*Uij*Astar(i)*Astar(j)), for Anisotropic Atoms

U(eq) = 1/3 Sum(i,j) (Uij*Astar(i)*Astar(j)*a(i).a(j))

Astar(i) are Reciprocal Axial Lengths and h(i) are Reflection Indices.

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Data on the Geometry of: C30H35Ti CP282

Table S4. Bond Distances (ang.) for: C30H35Ti CP282

Ti(1)	-C(1)	2.3657(17)	C(10)	-C(15)	1.395(2)
Ti(1)	-C(2)	2.3696(18)	C(11)	-C(12)	1.390(2)
Ti(1)	-C(3)	2.3793(17)	C(12)	-C(13)	1.383(2)
Ti(1)	-C(4)	2.3632(16)	C(13)	-C(14)	1.381(3)
Ti(1)	-C(5)	2.3418(15)	C(14)	-C(15)	1.390(2)
Ti(1)	-C(16)	2.3383(17)	C(16)	-C(17)	1.427(2)
Ti(1)	-C(17)	2.3696(17)	C(16)	-C(20)	1.426(2)
Ti(1)	-C(18)	2.3914(16)	C(16)	-C(21)	1.499(2)
Ti(1)	-C(19)	2.3896(16)	C(17)	-C(18)	1.411(2)
Ti(1)	-C(20)	2.3303(15)	C(17)	-C(22)	1.499(2)
C(1)	-C(2)	1.432(2)	C(18)	-C(19)	1.424(2)
C(1)	-C(5)	1.429(2)	C(18)	-C(23)	1.509(2)
C(1)	-C(6)	1.499(2)	C(19)	-C(20)	1.427(2)
C(2)	-C(3)	1.416(2)	C(19)	-C(24)	1.504(2)
C(2)	-C(7)	1.499(2)	C(20)	-C(25)	1.483(2)
C(3)	-C(4)	1.418(2)	C(25)	-C(26)	1.400(2)
C(3)	-C(8)	1.502(2)	C(25)	-C(30)	1.394(2)
C(4)	-C(5)	1.427(2)	C(26)	-C(27)	1.391(3)
C(4)	-C(9)	1.501(2)	C(27)	-C(28)	1.382(3)
C(5)	-C(10)	1.484(2)	C(28)	-C(29)	1.378(3)
C(10)	-C(11)	1.393(2)	C(29)	-C(30)	1.390(2)

-Hydrogen- parameters:

Ti(1)	-H(1)	1.768(15)	C(21)	-H(21)	0.96(2)
C(6)	-H(6)	0.986(18)	C(21)	-H(21')	0.97(2)
C(6)	-H(6')	0.929(19)	C(21)	-H(21")	0.92(2)
C(6)	-H(6")	0.976(18)	C(22)	-H(22)	1.02(2)
C(7)	-H(7)	0.94(2)	C(22)	-H(22')	0.89(2)
C(7)	-H(7')	0.94(2)	C(22)	-H(22")	0.99(2)
C(7)	-H(7")	0.98(2)	C(23)	-H(23)	0.976(19)
C(8)	-H(8)	0.923(19)	C(23)	-H(23')	0.95(2)
C(8)	-H(8')	0.98(2)	C(23)	-H(23")	0.95(2)
C(8)	-H(8")	0.96(2)	C(24)	-H(24)	0.896(19)
C(9)	-H(9)	0.92(2)	C(24)	-H(24')	1.027(18)
C(9)	-H(9')	1.00(2)	C(24)	-H(24")	0.953(19)
C(9)	-H(9")	0.87(2)	C(26)	-H(26)	1.005(17)
C(11)	-H(11)	0.965(18)	C(27)	-H(27)	0.922(19)
C(12)	-H(12)	0.977(18)	C(28)	-H(28)	0.968(19)
C(13)	-H(13)	0.982(19)	C(29)	-H(29)	0.983(18)
C(14)	-H(14)	0.986(19)	C(30)	-H(30)	0.943(17)
C(15)	-H(15)	0.979(19)			

Table S5. Angles (deg.) for: C30H35Ti CP282

C(1)	-Ti(1)	-C(2)	35.20(5)	C(2)	-C(3)	-C(4)	108.84(13)
C(1)	-Ti(1)	-C(3)	57.99(5)	C(2)	-C(3)	-C(8)	125.39(14)
C(1)	-Ti(1)	-C(4)	58.48(5)	C(4)	-C(3)	-C(8)	125.73(14)
C(1)	-Ti(1)	-C(5)	35.35(5)	Ti(1)	-C(4)	-C(3)	73.22(9)
C(1)	-Ti(1)	-C(16)	151.29(5)	Ti(1)	-C(4)	-C(5)	71.53(9)
C(1)	-Ti(1)	-C(17)	126.68(5)	Ti(1)	-C(4)	-C(9)	124.66(11)
C(1)	-Ti(1)	-C(18)	95.84(5)	C(3)	-C(4)	-C(5)	107.76(13)
C(1)	-Ti(1)	-C(19)	93.38(6)	C(3)	-C(4)	-C(9)	125.90(13)
C(1)	-Ti(1)	-C(20)	122.40(5)	C(5)	-C(4)	-C(9)	126.16(13)
C(2)	-Ti(1)	-C(3)	34.70(5)	Ti(1)	-C(5)	-C(1)	73.24(9)
C(2)	-Ti(1)	-C(4)	58.29(5)	Ti(1)	-C(5)	-C(4)	73.17(9)
C(2)	-Ti(1)	-C(5)	58.74(5)	Ti(1)	-C(5)	-C(10)	122.95(11)
C(2)	-Ti(1)	-C(16)	145.40(5)	C(1)	-C(5)	-C(4)	107.95(13)
C(2)	-Ti(1)	-C(17)	154.27(5)	C(1)	-C(5)	-C(10)	126.71(13)
C(2)	-Ti(1)	-C(18)	119.88(5)	C(4)	-C(5)	-C(10)	125.18(13)
C(2)	-Ti(1)	-C(19)	99.47(6)	C(5)	-C(10)	-C(11)	121.23(14)
C(2)	-Ti(1)	-C(20)	110.93(6)	C(5)	-C(10)	-C(15)	120.89(15)
C(3)	-Ti(1)	-C(4)	34.79(5)	C(11)	-C(10)	-C(15)	117.86(14)
C(3)	-Ti(1)	-C(5)	58.25(5)	C(10)	-C(11)	-C(12)	121.21(15)
C(3)	-Ti(1)	-C(16)	144.82(5)	C(11)	-C(12)	-C(13)	119.98(17)
C(3)	-Ti(1)	-C(17)	170.16(5)	C(12)	-C(13)	-C(14)	119.74(16)
C(3)	-Ti(1)	-C(18)	153.16(5)	C(13)	-C(14)	-C(15)	120.19(16)
C(3)	-Ti(1)	-C(19)	132.03(6)	C(10)	-C(15)	-C(14)	121.01(16)
C(3)	-Ti(1)	-C(20)	128.13(5)	Ti(1)	-C(16)	-C(17)	73.56(9)
C(4)	-Ti(1)	-C(5)	35.30(5)	Ti(1)	-C(16)	-C(20)	71.91(9)
C(4)	-Ti(1)	-C(16)	149.37(5)	Ti(1)	-C(16)	-C(21)	126.18(11)
C(4)	-Ti(1)	-C(17)	137.41(5)	C(17)	-C(16)	-C(20)	107.50(13)
C(4)	-Ti(1)	-C(18)	138.55(5)	C(17)	-C(16)	-C(21)	125.81(14)
C(4)	-Ti(1)	-C(19)	151.86(6)	C(20)	-C(16)	-C(21)	126.22(13)
C(4)	-Ti(1)	-C(20)	162.13(5)	Ti(1)	-C(17)	-C(16)	71.16(9)
C(5)	-Ti(1)	-C(16)	153.92(5)	Ti(1)	-C(17)	-C(18)	73.61(10)
C(5)	-Ti(1)	-C(17)	119.44(5)	Ti(1)	-C(17)	-C(22)	123.28(11)
C(5)	-Ti(1)	-C(18)	104.78(5)	C(16)	-C(17)	-C(18)	108.35(14)
C(5)	-Ti(1)	-C(19)	120.25(5)	C(16)	-C(17)	-C(22)	125.79(14)
C(5)	-Ti(1)	-C(20)	154.80(5)	C(18)	-C(17)	-C(22)	125.80(14)
C(16)	-Ti(1)	-C(17)	35.28(5)	Ti(1)	-C(18)	-C(17)	71.91(9)
C(16)	-Ti(1)	-C(18)	58.21(5)	Ti(1)	-C(18)	-C(19)	72.60(9)
C(16)	-Ti(1)	-C(19)	58.50(6)	Ti(1)	-C(18)	-C(23)	123.87(11)
C(16)	-Ti(1)	-C(20)	35.57(5)	C(17)	-C(18)	-C(19)	108.42(13)
C(17)	-Ti(1)	-C(18)	34.48(5)	C(17)	-C(18)	-C(23)	124.81(14)
C(17)	-Ti(1)	-C(19)	57.80(6)	C(19)	-C(18)	-C(23)	126.70(14)
C(17)	-Ti(1)	-C(20)	58.61(5)	Ti(1)	-C(19)	-C(18)	72.74(9)
C(18)	-Ti(1)	-C(19)	34.66(5)	Ti(1)	-C(19)	-C(20)	70.15(8)
C(18)	-Ti(1)	-C(20)	58.28(5)	Ti(1)	-C(19)	-C(24)	128.06(12)
C(19)	-Ti(1)	-C(20)	35.16(5)	C(18)	-C(19)	-C(20)	107.55(14)
Ti(1)	-C(1)	-C(2)	72.55(9)	C(18)	-C(19)	-C(24)	126.72(14)
Ti(1)	-C(1)	-C(5)	71.41(9)	C(20)	-C(19)	-C(24)	125.34(14)
Ti(1)	-C(1)	-C(6)	128.80(12)	Ti(1)	-C(20)	-C(16)	72.52(8)
C(2)	-C(1)	-C(5)	107.72(13)	Ti(1)	-C(20)	-C(19)	74.69(9)
C(2)	-C(1)	-C(6)	125.69(14)	Ti(1)	-C(20)	-C(25)	117.01(11)
C(5)	-C(1)	-C(6)	125.94(13)	C(16)	-C(20)	-C(19)	108.16(13)
Ti(1)	-C(2)	-C(1)	72.25(10)	C(16)	-C(20)	-C(25)	126.21(13)
Ti(1)	-C(2)	-C(3)	73.02(9)	C(19)	-C(20)	-C(25)	125.59(14)
Ti(1)	-C(2)	-C(7)	123.89(11)	C(20)	-C(25)	-C(26)	119.96(13)
C(1)	-C(2)	-C(3)	107.70(13)	C(20)	-C(25)	-C(30)	121.66(14)
C(1)	-C(2)	-C(7)	126.29(14)	C(26)	-C(25)	-C(30)	118.36(14)
C(3)	-C(2)	-C(7)	125.86(14)	C(25)	-C(26)	-C(27)	120.75(15)
Ti(1)	-C(3)	-C(2)	72.27(9)	C(26)	-C(27)	-C(28)	120.02(18)
Ti(1)	-C(3)	-C(4)	71.98(9)	C(27)	-C(28)	-C(29)	119.82(17)

-Hydrogen- parameters:

C(1)	-Ti(1)	-H(1)	133.5(5)	C(14)	-C(13)	-H(13)	121.6(12)
C(2)	-Ti(1)	-H(1)	113.1(6)	C(13)	-C(14)	-H(14)	120.4(11)
C(3)	-Ti(1)	-H(1)	79.9(6)	C(15)	-C(14)	-H(14)	119.4(11)
C(4)	-Ti(1)	-H(1)	75.8(5)	C(10)	-C(15)	-H(15)	117.9(10)
C(5)	-Ti(1)	-H(1)	107.0(5)	C(14)	-C(15)	-H(15)	121.1(10)
C(16)	-Ti(1)	-H(1)	75.3(5)	C(16)	-C(21)	-H(21)	114.3(13)
C(17)	-Ti(1)	-H(1)	92.3(5)	C(16)	-C(21)	-H(21')	108.5(12)
C(18)	-Ti(1)	-H(1)	126.7(5)	C(16)	-C(21)	-H(21")	113.5(13)
C(19)	-Ti(1)	-H(1)	131.9(5)	H(21)	-C(21)	-H(21')	109.6(17)
C(20)	-Ti(1)	-H(1)	98.2(5)	H(21)	-C(21)	-H(21")	102.2(18)
C(1)	-C(6)	-H(6)	111.9(10)	H(21')	-C(21)	-H(21")	108.4(17)
C(1)	-C(6)	-H(6')	113.7(12)	C(17)	-C(22)	-H(22)	113.9(11)
C(1)	-C(6)	-H(6")	112.9(11)	C(17)	-C(22)	-H(22')	110.5(13)
H(6)	-C(6)	-H(6')	103.8(16)	C(17)	-C(22)	-H(22")	111.1(14)
H(6)	-C(6)	-H(6")	104.9(15)	H(22)	-C(22)	-H(22')	103.2(18)
H(6')	-C(6)	-H(6")	108.8(16)	H(22)	-C(22)	-H(22")	107.1(17)
C(2)	-C(7)	-H(7)	110.7(12)	H(22')	-C(22)	-H(22")	111.(2)
C(2)	-C(7)	-H(7')	112.4(13)	C(18)	-C(23)	-H(23)	112.7(11)
C(2)	-C(7)	-H(7")	110.8(12)	C(18)	-C(23)	-H(23')	110.7(12)
H(7)	-C(7)	-H(7')	103.6(18)	C(18)	-C(23)	-H(23")	113.8(13)
H(7)	-C(7)	-H(7")	112.8(17)	H(23)	-C(23)	-H(23')	111.6(17)
H(7')	-C(7)	-H(7")	106.3(18)	H(23)	-C(23)	-H(23")	106.2(18)
C(3)	-C(8)	-H(8)	113.4(12)	H(23')	-C(23)	-H(23")	101.3(18)
C(3)	-C(8)	-H(8')	111.9(12)	C(19)	-C(24)	-H(24)	113.9(12)
C(3)	-C(8)	-H(8")	113.2(12)	C(19)	-C(24)	-H(24')	112.(1)
H(8)	-C(8)	-H(8')	106.7(17)	C(19)	-C(24)	-H(24")	113.6(11)
H(8)	-C(8)	-H(8")	101.1(17)	H(24)	-C(24)	-H(24')	105.1(15)
H(8')	-C(8)	-H(8")	109.9(18)	H(24)	-C(24)	-H(24")	105.3(17)
C(4)	-C(9)	-H(9)	111.0(13)	H(24')	-C(24)	-H(24")	106.1(15)
C(4)	-C(9)	-H(9')	113.5(12)	C(25)	-C(26)	-H(26)	120.1(10)
C(4)	-C(9)	-H(9")	114.4(14)	C(27)	-C(26)	-H(26)	119.1(10)
H(9)	-C(9)	-H(9')	111.5(17)	C(26)	-C(27)	-H(27)	118.1(11)
H(9)	-C(9)	-H(9")	104.0(19)	C(28)	-C(27)	-H(27)	121.9(11)
H(9')	-C(9)	-H(9")	101.7(18)	C(27)	-C(28)	-H(28)	120.0(12)
C(10)	-C(11)	-H(11)	119.7(11)	C(29)	-C(28)	-H(28)	120.2(12)
C(12)	-C(11)	-H(11)	119.1(11)	C(28)	-C(29)	-H(29)	122.3(11)
C(11)	-C(12)	-H(12)	120.4(10)	C(30)	-C(29)	-H(29)	117.0(11)
C(13)	-C(12)	-H(12)	119.6(10)	C(25)	-C(30)	-H(30)	120.5(10)
C(12)	-C(13)	-H(13)	118.7(12)	C(29)	-C(30)	-H(30)	119.1(10)

Table S6. Torsion Angles (deg.) for: C30H35Ti CP282

C(2)	-Ti(1)	-C(1)	-C(5)	116.25(13)	C(16)	-Ti(1)	-C(3)	-C(2)	-117.44(11)
C(2)	-Ti(1)	-C(1)	-C(6)	-122.13(17)	C(16)	-Ti(1)	-C(3)	-C(4)	125.14(10)
C(3)	-Ti(1)	-C(1)	-C(2)	-37.28(9)	C(16)	-Ti(1)	-C(3)	-C(8)	3.73(18)
C(3)	-Ti(1)	-C(1)	-C(5)	78.97(9)	C(18)	-Ti(1)	-C(3)	-C(2)	23.68(16)
C(3)	-Ti(1)	-C(1)	-C(6)	-159.41(16)	C(18)	-Ti(1)	-C(3)	-C(4)	-93.74(14)
C(4)	-Ti(1)	-C(1)	-C(2)	-78.45(9)	C(18)	-Ti(1)	-C(3)	-C(8)	144.86(12)
C(4)	-Ti(1)	-C(1)	-C(5)	37.80(9)	C(19)	-Ti(1)	-C(3)	-C(2)	-24.15(12)
C(4)	-Ti(1)	-C(1)	-C(6)	159.41(16)	C(19)	-Ti(1)	-C(3)	-C(4)	-141.56(9)
C(5)	-Ti(1)	-C(1)	-C(2)	-116.25(13)	C(19)	-Ti(1)	-C(3)	-C(8)	97.03(13)
C(5)	-Ti(1)	-C(1)	-C(6)	121.62(18)	C(20)	-Ti(1)	-C(3)	-C(2)	-70.38(10)
C(16)	-Ti(1)	-C(1)	-C(2)	112.62(12)	C(20)	-Ti(1)	-C(3)	-C(4)	172.20(8)
C(16)	-Ti(1)	-C(1)	-C(5)	-131.13(11)	C(20)	-Ti(1)	-C(3)	-C(8)	50.79(15)
C(16)	-Ti(1)	-C(1)	-C(6)	-9.5(2)	C(1)	-Ti(1)	-C(4)	-C(3)	78.04(9)
C(17)	-Ti(1)	-C(1)	-C(2)	153.22(8)	C(1)	-Ti(1)	-C(4)	-C(5)	-37.85(9)
C(17)	-Ti(1)	-C(1)	-C(5)	-90.53(10)	C(1)	-Ti(1)	-C(4)	-C(9)	-159.54(14)
C(17)	-Ti(1)	-C(1)	-C(6)	31.09(16)	C(2)	-Ti(1)	-C(4)	-C(3)	36.44(9)
C(18)	-Ti(1)	-C(1)	-C(2)	136.35(9)	C(2)	-Ti(1)	-C(4)	-C(5)	-79.45(10)
C(18)	-Ti(1)	-C(1)	-C(5)	-107.40(9)	C(2)	-Ti(1)	-C(4)	-C(9)	158.86(14)
C(18)	-Ti(1)	-C(1)	-C(6)	14.22(14)	C(3)	-Ti(1)	-C(4)	-C(5)	-115.89(13)
C(19)	-Ti(1)	-C(1)	-C(2)	101.65(9)	C(3)	-Ti(1)	-C(4)	-C(9)	122.42(16)
C(19)	-Ti(1)	-C(1)	-C(5)	-142.09(9)	C(5)	-Ti(1)	-C(4)	-C(3)	115.89(13)
C(19)	-Ti(1)	-C(1)	-C(6)	-20.48(14)	C(5)	-Ti(1)	-C(4)	-C(9)	-121.69(17)
C(20)	-Ti(1)	-C(1)	-C(2)	80.47(10)	C(16)	-Ti(1)	-C(4)	-C(3)	-112.39(12)
C(20)	-Ti(1)	-C(1)	-C(5)	-163.28(8)	C(16)	-Ti(1)	-C(4)	-C(5)	131.72(11)
C(20)	-Ti(1)	-C(1)	-C(6)	-41.66(16)	C(16)	-Ti(1)	-C(4)	-C(9)	10.03(19)
C(1)	-Ti(1)	-C(2)	-C(3)	-115.56(13)	C(17)	-Ti(1)	-C(4)	-C(3)	-170.36(9)
C(1)	-Ti(1)	-C(2)	-C(7)	122.25(16)	C(17)	-Ti(1)	-C(4)	-C(5)	73.75(12)
C(3)	-Ti(1)	-C(2)	-C(1)	115.56(13)	C(17)	-Ti(1)	-C(4)	-C(9)	-47.94(15)
C(3)	-Ti(1)	-C(2)	-C(7)	-122.19(16)	C(18)	-Ti(1)	-C(4)	-C(3)	137.11(10)
C(4)	-Ti(1)	-C(2)	-C(1)	79.02(9)	C(18)	-Ti(1)	-C(4)	-C(5)	21.22(13)
C(4)	-Ti(1)	-C(2)	-C(3)	-36.54(8)	C(18)	-Ti(1)	-C(4)	-C(9)	-100.47(13)
C(4)	-Ti(1)	-C(2)	-C(7)	-158.73(14)	C(19)	-Ti(1)	-C(4)	-C(3)	78.27(14)
C(5)	-Ti(1)	-C(2)	-C(1)	37.37(8)	C(19)	-Ti(1)	-C(4)	-C(5)	-37.62(16)
C(5)	-Ti(1)	-C(2)	-C(3)	-78.19(9)	C(19)	-Ti(1)	-C(4)	-C(9)	-159.31(12)
C(5)	-Ti(1)	-C(2)	-C(7)	159.62(14)	C(1)	-Ti(1)	-C(5)	-C(4)	115.30(13)
C(16)	-Ti(1)	-C(2)	-C(1)	-128.65(10)	C(1)	-Ti(1)	-C(5)	-C(10)	-123.29(15)
C(16)	-Ti(1)	-C(2)	-C(3)	115.79(11)	C(2)	-Ti(1)	-C(5)	-C(1)	-37.22(9)
C(16)	-Ti(1)	-C(2)	-C(7)	-6.40(18)	C(2)	-Ti(1)	-C(5)	-C(4)	78.08(10)
C(17)	-Ti(1)	-C(2)	-C(1)	-56.33(16)	C(2)	-Ti(1)	-C(5)	-C(10)	-160.51(13)
C(17)	-Ti(1)	-C(2)	-C(3)	-171.89(11)	C(3)	-Ti(1)	-C(5)	-C(1)	-78.16(10)
C(17)	-Ti(1)	-C(2)	-C(7)	65.92(18)	C(3)	-Ti(1)	-C(5)	-C(4)	37.13(9)
C(18)	-Ti(1)	-C(2)	-C(1)	-52.37(10)	C(3)	-Ti(1)	-C(5)	-C(10)	158.55(13)
C(18)	-Ti(1)	-C(2)	-C(3)	-167.93(8)	C(4)	-Ti(1)	-C(5)	-C(1)	-115.30(13)
C(18)	-Ti(1)	-C(2)	-C(7)	69.88(13)	C(4)	-Ti(1)	-C(5)	-C(10)	121.42(16)
C(19)	-Ti(1)	-C(2)	-C(1)	-82.38(9)	C(16)	-Ti(1)	-C(5)	-C(1)	124.60(13)
C(19)	-Ti(1)	-C(2)	-C(3)	162.06(9)	C(16)	-Ti(1)	-C(5)	-C(4)	-120.10(13)
C(19)	-Ti(1)	-C(2)	-C(7)	39.87(13)	C(16)	-Ti(1)	-C(5)	-C(10)	1.31(19)
C(20)	-Ti(1)	-C(2)	-C(1)	-116.94(9)	C(17)	-Ti(1)	-C(5)	-C(1)	112.95(9)
C(20)	-Ti(1)	-C(2)	-C(3)	127.50(9)	C(17)	-Ti(1)	-C(5)	-C(4)	-131.76(9)
C(20)	-Ti(1)	-C(2)	-C(7)	5.31(14)	C(17)	-Ti(1)	-C(5)	-C(10)	-10.34(13)
C(1)	-Ti(1)	-C(3)	-C(2)	37.83(9)	C(18)	-Ti(1)	-C(5)	-C(1)	79.05(10)
C(1)	-Ti(1)	-C(3)	-C(4)	-79.58(9)	C(18)	-Ti(1)	-C(5)	-C(4)	-165.66(9)
C(1)	-Ti(1)	-C(3)	-C(8)	159.01(14)	C(18)	-Ti(1)	-C(5)	-C(10)	-44.24(12)
C(2)	-Ti(1)	-C(3)	-C(4)	-117.42(13)	C(19)	-Ti(1)	-C(5)	-C(1)	45.24(11)
C(2)	-Ti(1)	-C(3)	-C(8)	121.18(16)	C(19)	-Ti(1)	-C(5)	-C(4)	160.53(9)
C(4)	-Ti(1)	-C(3)	-C(2)	117.42(13)	C(19)	-Ti(1)	-C(5)	-C(10)	-78.05(13)
C(4)	-Ti(1)	-C(3)	-C(8)	-121.41(16)	C(20)	-Ti(1)	-C(5)	-C(1)	34.80(17)
C(5)	-Ti(1)	-C(3)	-C(2)	79.73(9)	C(20)	-Ti(1)	-C(5)	-C(4)	150.10(13)
C(5)	-Ti(1)	-C(3)	-C(4)	-37.69(8)	C(20)	-Ti(1)	-C(5)	-C(10)	-88.49(17)

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C(1)	-Ti(1)	-C(16)	-C(20)	-50.56(15)
C(1)	-Ti(1)	-C(16)	-C(21)	-172.65(12)
C(2)	-Ti(1)	-C(16)	-C(17)	134.25(10)
C(2)	-Ti(1)	-C(16)	-C(20)	19.02(14)
C(2)	-Ti(1)	-C(16)	-C(21)	-103.07(15)
C(3)	-Ti(1)	-C(16)	-C(17)	-162.91(9)
C(3)	-Ti(1)	-C(16)	-C(20)	81.87(12)
C(3)	-Ti(1)	-C(16)	-C(21)	-40.22(18)
C(4)	-Ti(1)	-C(16)	-C(17)	-96.59(12)
C(4)	-Ti(1)	-C(16)	-C(20)	148.18(10)
C(4)	-Ti(1)	-C(16)	-C(21)	26.09(19)
C(5)	-Ti(1)	-C(16)	-C(17)	-17.73(16)
C(5)	-Ti(1)	-C(16)	-C(20)	-132.96(12)
C(5)	-Ti(1)	-C(16)	-C(21)	104.95(15)
C(17)	-Ti(1)	-C(16)	-C(20)	-115.23(12)
C(17)	-Ti(1)	-C(16)	-C(21)	122.68(17)
C(18)	-Ti(1)	-C(16)	-C(17)	36.57(9)
C(18)	-Ti(1)	-C(16)	-C(20)	-78.66(9)
C(18)	-Ti(1)	-C(16)	-C(21)	159.25(15)
C(19)	-Ti(1)	-C(16)	-C(17)	77.53(9)
C(19)	-Ti(1)	-C(16)	-C(20)	-37.69(8)
C(19)	-Ti(1)	-C(16)	-C(21)	-159.78(15)
C(20)	-Ti(1)	-C(16)	-C(17)	115.23(12)
C(20)	-Ti(1)	-C(16)	-C(21)	-122.09(16)
C(1)	-Ti(1)	-C(17)	-C(16)	-147.22(9)
C(1)	-Ti(1)	-C(17)	-C(18)	-30.67(11)
C(1)	-Ti(1)	-C(17)	-C(22)	91.76(13)
C(2)	-Ti(1)	-C(17)	-C(16)	-110.48(13)
C(2)	-Ti(1)	-C(17)	-C(18)	6.08(17)
C(2)	-Ti(1)	-C(17)	-C(22)	128.51(14)
C(4)	-Ti(1)	-C(17)	-C(16)	131.59(9)
C(4)	-Ti(1)	-C(17)	-C(18)	-111.86(10)
C(4)	-Ti(1)	-C(17)	-C(22)	10.57(16)
C(5)	-Ti(1)	-C(17)	-C(16)	171.16(8)
C(5)	-Ti(1)	-C(17)	-C(18)	-72.29(10)
C(5)	-Ti(1)	-C(17)	-C(22)	50.14(14)
C(16)	-Ti(1)	-C(17)	-C(18)	116.55(13)
C(16)	-Ti(1)	-C(17)	-C(22)	-121.02(16)
C(18)	-Ti(1)	-C(17)	-C(16)	-116.55(13)
C(18)	-Ti(1)	-C(17)	-C(22)	122.43(16)
C(19)	-Ti(1)	-C(17)	-C(16)	-79.68(9)
C(19)	-Ti(1)	-C(17)	-C(18)	36.87(8)
C(19)	-Ti(1)	-C(17)	-C(22)	159.30(15)
C(20)	-Ti(1)	-C(17)	-C(16)	-38.06(8)
C(20)	-Ti(1)	-C(17)	-C(18)	78.50(9)
C(20)	-Ti(1)	-C(17)	-C(22)	-159.08(15)
C(1)	-Ti(1)	-C(18)	-C(17)	155.72(9)
C(1)	-Ti(1)	-C(18)	-C(19)	-87.49(10)
C(1)	-Ti(1)	-C(18)	-C(23)	35.45(14)
C(2)	-Ti(1)	-C(18)	-C(17)	-176.96(8)
C(2)	-Ti(1)	-C(18)	-C(19)	-60.17(11)
C(2)	-Ti(1)	-C(18)	-C(23)	62.77(15)
C(3)	-Ti(1)	-C(18)	-C(17)	167.75(11)
C(3)	-Ti(1)	-C(18)	-C(19)	-75.46(15)
C(3)	-Ti(1)	-C(18)	-C(23)	47.5(2)
C(4)	-Ti(1)	-C(18)	-C(17)	108.41(10)
C(4)	-Ti(1)	-C(18)	-C(19)	-134.8(1)
C(4)	-Ti(1)	-C(18)	-C(23)	-11.85(18)
C(5)	-Ti(1)	-C(18)	-C(17)	120.90(9)
C(5)	-Ti(1)	-C(18)	-C(19)	-122.31(9)
C(5)	-Ti(1)	-C(18)	-C(23)	0.64(14)
C(16)	-Ti(1)	-C(18)	-C(17)	-37.43(9)
C(16)	-Ti(1)	-C(18)	-C(23)	-157.69(15)
C(17)	-Ti(1)	-C(18)	-C(19)	116.79(13)
C(17)	-Ti(1)	-C(18)	-C(23)	-120.27(17)
C(19)	-Ti(1)	-C(18)	-C(17)	-116.79(13)
C(19)	-Ti(1)	-C(18)	-C(23)	122.95(18)
C(20)	-Ti(1)	-C(18)	-C(17)	-79.53(9)
C(20)	-Ti(1)	-C(18)	-C(19)	37.25(9)
C(20)	-Ti(1)	-C(18)	-C(23)	160.20(16)
C(1)	-Ti(1)	-C(19)	-C(18)	95.39(10)
C(1)	-Ti(1)	-C(19)	-C(20)	-148.01(10)
C(1)	-Ti(1)	-C(19)	-C(24)	-28.11(13)
C(2)	-Ti(1)	-C(19)	-C(18)	130.30(9)
C(2)	-Ti(1)	-C(19)	-C(20)	-113.09(10)
C(2)	-Ti(1)	-C(19)	-C(24)	6.81(14)
C(3)	-Ti(1)	-C(19)	-C(18)	143.96(9)
C(3)	-Ti(1)	-C(19)	-C(20)	-99.43(11)
C(3)	-Ti(1)	-C(19)	-C(24)	20.46(16)
C(4)	-Ti(1)	-C(19)	-C(18)	95.19(14)
C(4)	-Ti(1)	-C(19)	-C(20)	-148.21(12)
C(4)	-Ti(1)	-C(19)	-C(24)	-28.3(2)
C(5)	-Ti(1)	-C(19)	-C(18)	71.09(11)
C(5)	-Ti(1)	-C(19)	-C(20)	-172.31(9)
C(5)	-Ti(1)	-C(19)	-C(24)	-52.41(15)
C(16)	-Ti(1)	-C(19)	-C(18)	-78.46(10)
C(16)	-Ti(1)	-C(19)	-C(20)	38.14(9)
C(16)	-Ti(1)	-C(19)	-C(24)	158.04(15)
C(17)	-Ti(1)	-C(19)	-C(18)	-36.67(9)
C(17)	-Ti(1)	-C(19)	-C(20)	79.93(10)
C(17)	-Ti(1)	-C(19)	-C(24)	-160.17(15)
C(18)	-Ti(1)	-C(19)	-C(20)	116.60(14)
C(18)	-Ti(1)	-C(19)	-C(24)	-123.50(17)
C(20)	-Ti(1)	-C(19)	-C(18)	-116.60(14)
C(20)	-Ti(1)	-C(19)	-C(24)	119.90(17)
C(1)	-Ti(1)	-C(20)	-C(16)	153.93(8)
C(1)	-Ti(1)	-C(20)	-C(19)	38.78(12)
C(1)	-Ti(1)	-C(20)	-C(25)	-83.74(12)
C(2)	-Ti(1)	-C(20)	-C(16)	-168.57(8)
C(2)	-Ti(1)	-C(20)	-C(19)	76.28(10)
C(2)	-Ti(1)	-C(20)	-C(25)	-46.25(12)
C(3)	-Ti(1)	-C(20)	-C(16)	-133.53(9)
C(3)	-Ti(1)	-C(20)	-C(19)	111.32(10)
C(3)	-Ti(1)	-C(20)	-C(25)	-11.21(14)
C(5)	-Ti(1)	-C(20)	-C(16)	130.91(13)
C(5)	-Ti(1)	-C(20)	-C(19)	15.76(18)
C(5)	-Ti(1)	-C(20)	-C(25)	-106.76(15)
C(16)	-Ti(1)	-C(20)	-C(19)	-115.15(13)
C(16)	-Ti(1)	-C(20)	-C(25)	122.32(15)
C(17)	-Ti(1)	-C(20)	-C(16)	37.74(8)
C(17)	-Ti(1)	-C(20)	-C(19)	-77.42(10)
C(17)	-Ti(1)	-C(20)	-C(25)	160.06(13)
C(18)	-Ti(1)	-C(20)	-C(16)	78.44(9)
C(18)	-Ti(1)	-C(20)	-C(19)	-36.71(9)
C(18)	-Ti(1)	-C(20)	-C(25)	-159.24(13)
C(19)	-Ti(1)	-C(20)	-C(16)	115.15(13)
C(19)	-Ti(1)	-C(20)	-C(25)	-122.53(16)
Ti(1)	-C(1)	-C(2)	-C(3)	64.91(12)
Ti(1)	-C(1)	-C(2)	-C(7)	-119.42(17)
C(5)	-C(1)	-C(2)	-Ti(1)	-63.18(11)
C(5)	-C(1)	-C(2)	-C(3)	1.74(19)
C(5)	-C(1)	-C(2)	-C(7)	177.40(16)
C(6)	-C(1)	-C(2)	-Ti(1)	125.66(17)
C(6)	-C(1)	-C(2)	-C(3)	-169.43(16)

Ti(1)	-C(1)	-C(5)	-C(4)	-65.46(11)
Ti(1)	-C(1)	-C(5)	-C(10)	118.95(17)
C(2)	-C(1)	-C(5)	-Ti(1)	63.92(12)
C(2)	-C(1)	-C(5)	-C(4)	-1.54(19)
C(2)	-C(1)	-C(5)	-C(10)	-177.14(16)
C(6)	-C(1)	-C(5)	-Ti(1)	-124.95(17)
C(6)	-C(1)	-C(5)	-C(4)	169.60(16)
C(6)	-C(1)	-C(5)	-C(10)	-6.0(3)
Ti(1)	-C(2)	-C(3)	-C(4)	63.12(12)
Ti(1)	-C(2)	-C(3)	-C(8)	-119.03(16)
C(1)	-C(2)	-C(3)	-Ti(1)	-64.40(12)
C(1)	-C(2)	-C(3)	-C(4)	-1.28(19)
C(1)	-C(2)	-C(3)	-C(8)	176.57(16)
C(7)	-C(2)	-C(3)	-Ti(1)	119.91(17)
C(7)	-C(2)	-C(3)	-C(4)	-176.97(16)
C(7)	-C(2)	-C(3)	-C(8)	0.9(3)
Ti(1)	-C(3)	-C(4)	-C(5)	63.64(11)
Ti(1)	-C(3)	-C(4)	-C(9)	-121.00(17)
C(2)	-C(3)	-C(4)	-Ti(1)	-63.31(12)
C(2)	-C(3)	-C(4)	-C(5)	0.33(19)
C(2)	-C(3)	-C(4)	-C(9)	175.70(16)
C(8)	-C(3)	-C(4)	-Ti(1)	118.85(16)
C(8)	-C(3)	-C(4)	-C(5)	-177.51(15)
C(8)	-C(3)	-C(4)	-C(9)	-2.1(3)
Ti(1)	-C(4)	-C(5)	-C(1)	65.50(11)
Ti(1)	-C(4)	-C(5)	-C(10)	-118.81(16)
C(3)	-C(4)	-C(5)	-Ti(1)	-64.75(11)
C(3)	-C(4)	-C(5)	-C(1)	0.75(19)
C(3)	-C(4)	-C(5)	-C(10)	176.44(15)
C(9)	-C(4)	-C(5)	-Ti(1)	119.90(17)
C(9)	-C(4)	-C(5)	-C(1)	-174.60(16)
C(9)	-C(4)	-C(5)	-C(10)	1.1(3)
Ti(1)	-C(5)	-C(10)	-C(11)	-40.93(19)
Ti(1)	-C(5)	-C(10)	-C(15)	140.63(13)
C(1)	-C(5)	-C(10)	-C(11)	-134.07(18)
C(1)	-C(5)	-C(10)	-C(15)	47.5(2)
C(4)	-C(5)	-C(10)	-C(11)	51.1(2)
C(4)	-C(5)	-C(10)	-C(15)	-127.38(18)
C(5)	-C(10)	-C(11)	-C(12)	-178.83(16)
C(15)	-C(10)	-C(11)	-C(12)	-0.3(2)
C(5)	-C(10)	-C(15)	-C(14)	179.04(15)
C(11)	-C(10)	-C(15)	-C(14)	0.6(2)
C(10)	-C(11)	-C(12)	-C(13)	-0.3(3)
C(11)	-C(12)	-C(13)	-C(14)	0.8(3)
C(12)	-C(13)	-C(14)	-C(15)	-0.6(3)
C(13)	-C(14)	-C(15)	-C(10)	-0.1(3)
Ti(1)	-C(16)	-C(17)	-C(18)	-64.70(12)
Ti(1)	-C(16)	-C(17)	-C(22)	117.96(16)
C(20)	-C(16)	-C(17)	-Ti(1)	64.38(11)
C(20)	-C(16)	-C(17)	-C(18)	-0.3(2)
C(20)	-C(16)	-C(17)	-C(22)	-177.67(16)
C(21)	-C(16)	-C(17)	-Ti(1)	-123.09(16)
C(21)	-C(16)	-C(17)	-C(18)	172.20(16)
C(21)	-C(16)	-C(17)	-C(22)	-5.1(3)
Ti(1)	-C(16)	-C(20)	-C(19)	66.75(11)
Ti(1)	-C(16)	-C(20)	-C(25)	-111.07(16)
C(17)	-C(16)	-C(20)	-Ti(1)	-65.47(11)
C(17)	-C(16)	-C(20)	-C(19)	1.28(18)
C(17)	-C(16)	-C(20)	-C(25)	-176.54(15)
C(21)	-C(16)	-C(20)	-Ti(1)	122.04(17)
C(21)	-C(16)	-C(20)	-C(19)	-171.21(16)
C(21)	-C(16)	-C(20)	-C(25)	11.0(3)
Ti(1)	-C(17)	-C(18)	-C(19)	-63.87(12)
Ti(1)	-C(17)	-C(18)	-C(23)	119.15(16)
C(16)	-C(17)	-C(18)	-Ti(1)	63.12(11)
C(16)	-C(17)	-C(18)	-C(19)	-0.76(18)
C(16)	-C(17)	-C(18)	-C(23)	-177.73(16)
C(22)	-C(17)	-C(18)	-Ti(1)	-119.54(17)
C(22)	-C(17)	-C(18)	-C(19)	176.59(16)
C(22)	-C(17)	-C(18)	-C(23)	-0.4(3)
Ti(1)	-C(18)	-C(19)	-C(20)	-61.89(11)
Ti(1)	-C(18)	-C(19)	-C(24)	125.00(18)
C(17)	-C(18)	-C(19)	-Ti(1)	63.43(12)
C(17)	-C(18)	-C(19)	-C(20)	1.54(19)
C(17)	-C(18)	-C(19)	-C(24)	-171.57(16)
C(23)	-C(18)	-C(19)	-Ti(1)	-119.66(17)
C(23)	-C(18)	-C(19)	-C(20)	178.45(16)
C(23)	-C(18)	-C(19)	-C(24)	5.3(3)
Ti(1)	-C(19)	-C(20)	-C(16)	-65.32(11)
Ti(1)	-C(19)	-C(20)	-C(25)	112.53(16)
C(18)	-C(19)	-C(20)	-Ti(1)	63.57(11)
C(18)	-C(19)	-C(20)	-C(16)	-1.74(18)
C(18)	-C(19)	-C(20)	-C(25)	176.10(15)
C(24)	-C(19)	-C(20)	-Ti(1)	-123.20(17)
C(24)	-C(19)	-C(20)	-C(16)	171.49(16)
C(24)	-C(19)	-C(20)	-C(25)	-10.7(3)
Ti(1)	-C(20)	-C(25)	-C(26)	-34.6(2)
Ti(1)	-C(20)	-C(25)	-C(30)	143.85(14)
C(16)	-C(20)	-C(25)	-C(26)	52.8(2)
C(16)	-C(20)	-C(25)	-C(30)	-128.71(18)
C(19)	-C(20)	-C(25)	-C(26)	-124.66(18)
C(19)	-C(20)	-C(25)	-C(30)	53.8(2)
C(20)	-C(25)	-C(26)	-C(27)	177.36(17)
C(30)	-C(25)	-C(26)	-C(27)	-1.2(3)
C(20)	-C(25)	-C(30)	-C(29)	-177.10(17)
C(26)	-C(25)	-C(30)	-C(29)	1.4(3)
C(25)	-C(26)	-C(27)	-C(28)	0.0(3)
C(26)	-C(27)	-C(28)	-C(29)	1.0(3)
C(27)	-C(28)	-C(29)	-C(30)	-0.7(3)
C(28)	-C(29)	-C(30)	-C(25)	-0.5(3)

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-Hydrogen- parameters:

H(1)	-Ti(1)	-C(1)	-C(2)	-66.0(7)	C(3)	-C(4)	-C(9)	-H(9")	-13.6(15)
H(1)	-Ti(1)	-C(1)	-C(5)	50.3(7)	C(5)	-C(4)	-C(9)	-H(9)	43.5(14)
H(1)	-Ti(1)	-C(1)	-C(6)	171.9(7)	C(5)	-C(4)	-C(9)	-H(9')	-82.9(13)
H(1)	-Ti(1)	-C(2)	-C(1)	133.9(5)	C(5)	-C(4)	-C(9)	-H(9")	160.9(15)
H(1)	-Ti(1)	-C(2)	-C(3)	18.3(5)	C(5)	-C(10)	-C(11)	-H(11)	1.8(12)
H(1)	-Ti(1)	-C(2)	-C(7)	-103.9(5)	C(15)	-C(10)	-C(11)	-H(11)	-179.7(12)
H(1)	-Ti(1)	-C(3)	-C(2)	-162.9(5)	C(5)	-C(10)	-C(15)	-H(15)	-0.2(11)
H(1)	-Ti(1)	-C(3)	-C(4)	79.7(5)	C(11)	-C(10)	-C(15)	-H(15)	-178.7(12)
H(1)	-Ti(1)	-C(3)	-C(8)	-41.7(5)	C(10)	-C(11)	-C(12)	-H(12)	178.2(12)
H(1)	-Ti(1)	-C(4)	-C(3)	-92.7(5)	H(11)	-C(11)	-C(12)	-C(13)	179.1(12)
H(1)	-Ti(1)	-C(4)	-C(5)	151.4(5)	H(11)	-C(11)	-C(12)	-H(12)	-2.5(17)
H(1)	-Ti(1)	-C(4)	-C(9)	29.8(5)	C(11)	-C(12)	-C(13)	-H(13)	-179.6(13)
H(1)	-Ti(1)	-C(5)	-C(1)	-144.3(6)	H(12)	-C(12)	-C(13)	-C(14)	-177.7(11)
H(1)	-Ti(1)	-C(5)	-C(4)	-29.0(6)	H(12)	-C(12)	-C(13)	-H(13)	1.9(17)
H(1)	-Ti(1)	-C(5)	-C(10)	92.4(6)	C(12)	-C(13)	-C(14)	-H(14)	178.0(13)
H(1)	-Ti(1)	-C(16)	-C(17)	-116.4(5)	H(13)	-C(13)	-C(14)	-C(15)	179.9(12)
H(1)	-Ti(1)	-C(16)	-C(20)	128.4(5)	H(13)	-C(13)	-C(14)	-H(14)	-1.5(18)
H(1)	-Ti(1)	-C(16)	-C(21)	6.3(5)	C(13)	-C(14)	-C(15)	-H(15)	179.2(13)
H(1)	-Ti(1)	-C(17)	-C(16)	60.1(5)	H(14)	-C(14)	-C(15)	-C(10)	-178.7(13)
H(1)	-Ti(1)	-C(17)	-C(18)	176.7(5)	H(14)	-C(14)	-C(15)	-H(15)	0.5(18)
H(1)	-Ti(1)	-C(17)	-C(22)	-60.9(5)	Ti(1)	-C(16)	-C(21)	-H(21)	55.1(14)
H(1)	-Ti(1)	-C(18)	-C(17)	-4.1(6)	Ti(1)	-C(16)	-C(21)	-H(21')	177.7(12)
H(1)	-Ti(1)	-C(18)	-C(19)	112.7(6)	Ti(1)	-C(16)	-C(21)	-H(21")	-61.7(14)
H(1)	-Ti(1)	-C(18)	-C(23)	-124.4(6)	C(17)	-C(16)	-C(21)	-H(21)	150.5(14)
H(1)	-Ti(1)	-C(19)	-C(18)	-96.6(7)	C(17)	-C(16)	-C(21)	-H(21')	-86.8(12)
H(1)	-Ti(1)	-C(19)	-C(20)	20.0(7)	C(17)	-C(16)	-C(21)	-H(21")	33.8(14)
H(1)	-Ti(1)	-C(19)	-C(24)	139.9(7)	C(20)	-C(16)	-C(21)	-H(21)	-38.3(14)
H(1)	-Ti(1)	-C(20)	-C(16)	-50.0(5)	C(20)	-C(16)	-C(21)	-H(21')	84.3(12)
H(1)	-Ti(1)	-C(20)	-C(19)	-165.1(5)	C(20)	-C(16)	-C(21)	-H(21")	-155.1(14)
H(1)	-Ti(1)	-C(20)	-C(25)	72.4(5)	Ti(1)	-C(17)	-C(22)	-H(22)	-63.8(12)
Ti(1)	-C(1)	-C(6)	-H(6)	-176.3(11)	Ti(1)	-C(17)	-C(22)	-H(22')	-179.3(14)
Ti(1)	-C(1)	-C(6)	-H(6')	66.4(14)	Ti(1)	-C(17)	-C(22)	-H(22")	57.3(16)
Ti(1)	-C(1)	-C(6)	-H(6")	-58.2(11)	C(16)	-C(17)	-C(22)	-H(22)	-153.6(12)
C(2)	-C(1)	-C(6)	-H(6)	87.7(11)	C(16)	-C(17)	-C(22)	-H(22')	90.9(14)
C(2)	-C(1)	-C(6)	-H(6')	-29.5(14)	C(16)	-C(17)	-C(22)	-H(22")	-32.5(16)
C(2)	-C(1)	-C(6)	-H(6")	-154.2(11)	C(18)	-C(17)	-C(22)	-H(22)	29.5(12)
C(5)	-C(1)	-C(6)	-H(6)	-81.8(11)	C(18)	-C(17)	-C(22)	-H(22')	-86.0(14)
C(5)	-C(1)	-C(6)	-H(6')	160.9(14)	C(18)	-C(17)	-C(22)	-H(22")	150.6(16)
C(5)	-C(1)	-C(6)	-H(6")	36.3(11)	Ti(1)	-C(18)	-C(23)	-H(23)	26.1(13)
Ti(1)	-C(2)	-C(7)	-H(7)	-73.2(13)	Ti(1)	-C(18)	-C(23)	-H(23')	151.8(13)
Ti(1)	-C(2)	-C(7)	-H(7')	171.5(14)	Ti(1)	-C(18)	-C(23)	-H(23")	-94.9(14)
Ti(1)	-C(2)	-C(7)	-H(7")	52.7(13)	C(17)	-C(18)	-C(23)	-H(23)	-64.6(13)
C(1)	-C(2)	-C(7)	-H(7)	19.0(13)	C(17)	-C(18)	-C(23)	-H(23')	61.2(14)
C(1)	-C(2)	-C(7)	-H(7')	-96.4(14)	C(17)	-C(18)	-C(23)	-H(23")	174.5(14)
C(1)	-C(2)	-C(7)	-H(7")	144.9(13)	C(19)	-C(18)	-C(23)	-H(23)	119.0(13)
C(3)	-C(2)	-C(7)	-H(7)	-166.1(13)	C(19)	-C(18)	-C(23)	-H(23')	-115.2(14)
C(3)	-C(2)	-C(7)	-H(7')	78.5(14)	C(19)	-C(18)	-C(23)	-H(23")	-1.9(15)
C(3)	-C(2)	-C(7)	-H(7")	-40.2(13)	Ti(1)	-C(19)	-C(24)	-H(24)	71.0(14)
Ti(1)	-C(3)	-C(8)	-H(8)	-69.4(14)	Ti(1)	-C(19)	-C(24)	-H(24')	-169.9(10)
Ti(1)	-C(3)	-C(8)	-H(8')	51.4(13)	Ti(1)	-C(19)	-C(24)	-H(24")	-49.7(12)
Ti(1)	-C(3)	-C(8)	-H(8")	176.2(13)	C(18)	-C(19)	-C(24)	-H(24)	-25.6(14)
C(2)	-C(3)	-C(8)	-H(8)	21.9(14)	C(18)	-C(19)	-C(24)	-H(24')	93.5(10)
C(2)	-C(3)	-C(8)	-H(8')	142.7(13)	C(18)	-C(19)	-C(24)	-H(24")	-146.2(12)
C(2)	-C(3)	-C(8)	-H(8")	-92.5(14)	C(20)	-C(19)	-C(24)	-H(24)	162.5(14)
C(4)	-C(3)	-C(8)	-H(8)	-160.6(14)	C(20)	-C(19)	-C(24)	-H(24')	-78.4(10)
C(4)	-C(3)	-C(8)	-H(8')	-39.8(13)	C(20)	-C(19)	-C(24)	-H(24")	41.9(12)
C(4)	-C(3)	-C(8)	-H(8")	85.0(14)	C(20)	-C(25)	-C(26)	-H(26)	-0.9(11)
Ti(1)	-C(4)	-C(9)	-H(9)	135.2(14)	C(30)	-C(25)	-C(26)	-H(26)	-179.4(13)
Ti(1)	-C(4)	-C(9)	-H(9')	8.7(13)	C(20)	-C(25)	-C(30)	-H(30)	4.7(13)
Ti(1)	-C(4)	-C(9)	-H(9")	-107.4(15)	C(26)	-C(25)	-C(30)	-H(30)	-176.8(13)
C(3)	-C(4)	-C(9)	-H(9)	-131.0(14)	C(25)	-C(26)	-C(27)	-H(27)	-178.7(14)

H(26)	-C(26)	-C(27)	-H(27)	-0.4(17)	H(28)	-C(28)	-C(29)	-C(30)	176.6(14)
C(26)	-C(27)	-C(28)	-H(28)	-176.4(14)	H(28)	-C(28)	-C(29)	-H(29)	-2.9(19)
H(27)	-C(27)	-C(28)	-C(29)	179.6(16)	C(28)	-C(29)	-C(30)	-H(30)	177.8(13)
H(27)	-C(27)	-C(28)	-H(28)	2.(2)	H(29)	-C(29)	-C(30)	-C(25)	179.0(13)
C(27)	-C(28)	-C(29)	-H(29)	179.8(10)	H(29)	-C(29)	-C(30)	-H(30)	-2.7(18)

The sign of the torsion angle is positive if when looking from atom-2 to atom-3 a clockwise motion of atom-1 would superimpose it on atom-4.